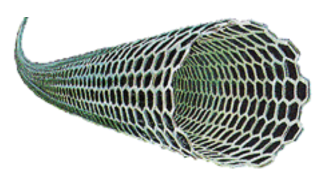
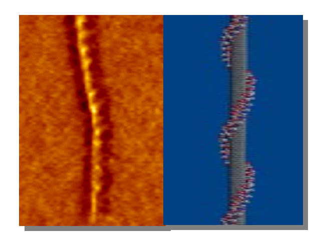
Molecular Spectroscopy of Carbon Nanotubes
M.S. Dresselhaus MIT; DMR 0405538

Education:
4 graduate students (Georgii Samsonidze, S. Grace Chou, Hyongbin Son, Daniel Nezich), 1 undergraduate (Victor Brar) and a visiting graduate student (Eduardo Barros from the Federal University of Ceara, Brazil) worked collaboratively on the molecular spectroscopy of carbon nanotubes grant, making numerous scientific advances documented in scientific publications and presentations at national and international conferences. In 2004 Georgii Samsonidze spent 1 month in Japan and S. Grace Chou spent 6 weeks (on two trips) in Brazil working with foreign collaborators.
During the summer, our research group hosted a high school student (Lahari Koganti from India) who learned how to do Raman scattering on nanotubes.

Outreach:
When the PI gives colloquia at other universities (about once per month), she also carries out mentoring and facilitation sessions (usually as a breakfast or lunch meeting) with graduate students and postdocs to guide them in their careers. In addition, she gives invited talks (about 10/yr) at museums (such as the Boston Museum of Science as shown below) or at science conferences (such as the XIII International Materials Research Conference in Cancun, Mexico, August 24, 2004) or more generally (such as the Conference on Mentoring young Scientists in Vienna, Austria, Nov. 7, 2003)

Exciting Opportunities for Women in Nanoscience and Nanotechnology
Mildred Dresselhaus
Women in Science Lunch at the Science Museum, Boston, MA
May 12, 2004

Opening viewgraph showing model of a carbon nanotube (left) and a DNA wrapped nanotube (right).

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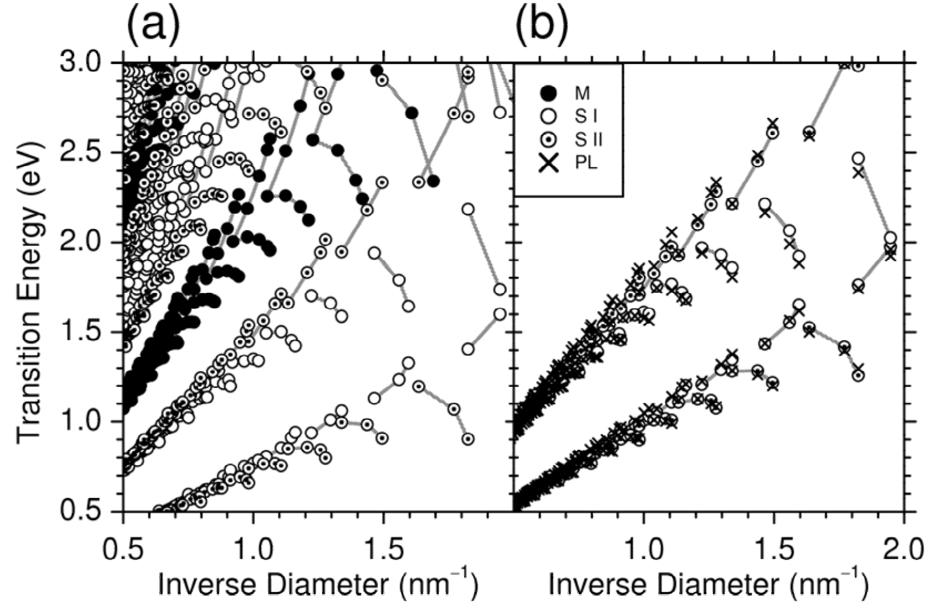
The objective of this work is to explain the recently discovered family behavior in the experimental "Kataura" plot based on photoluminescence data [R. B. Weisman & S. M. Bachilo, Nano Lett. **3**, 1235 (2003)]

Using Popov's extension of the tight-binding model that allows bond lengths and angles to vary, we have calculated the optical transition energies E_{ii} in single-wall carbon nanotubes (SWNTs), as a function of inverse tube diameter. After geometrical structural optimization, the 2n+m=constant family structure observed in photoluminescence (PL) experiments is obtained, and detailed agreement between the calculations, PL experiments and Resonance Raman spectra is achieved after including many-body corrections. These findings open new directions for exploring the molecular spectroscopy of individual SWNTs.



(a) "Kataura" plot of transition energies E_{ii} vs. $1/d_t$ for semiconducting and metallic SWNTs based on Popov's tight binding model after geometrical structure optimization. (b) Comparison showing excellent agreement between PL experimental data and calculations in (a) for E_{11}^S and E_{22}^S, and after making many-body corrections.

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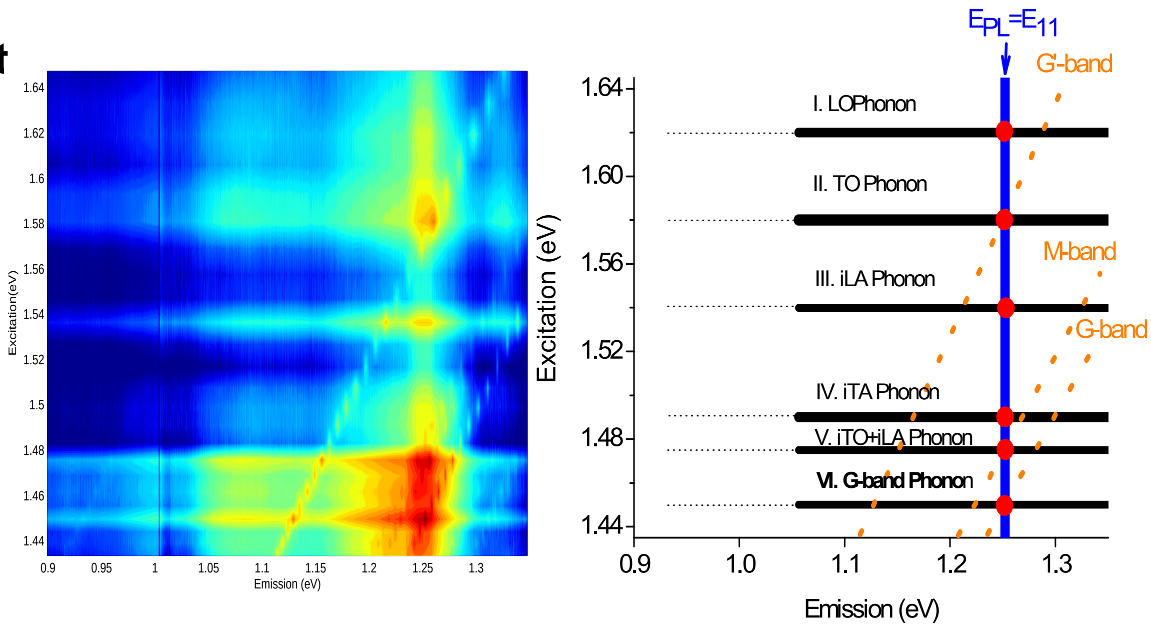
Research Summary:

In this study, photoluminescence (PL) measurements were carried out on DNA-wrapped nanotubes. Using a sample of DNA-wrapped single wall carbon nanotubes strongly enriched in the (6,5) nanotubes, the PL emissions for special excitation energy values were identified with specific mechanisms of electron and hole relaxation associated with (6,5) nanotubes, including one phonon, two phonon, hot luminescence processes, as well as radiative and non-radiative energy transferring processes between neighboring nanotubes. Such relaxation processes are not separately identified in general condensed matter physics studies on three dimensional crystalline systems.

2D excitation vs. emission map (left) and schematics for a (6,5) enriched DNA-wrapped nanotube sample (right)



- Blue vertical line denotes emission at the band edge.
- Orange dotted lines denote PL emission from Raman processes for special phonons.
- Strong PL spots, denoted by the red circles I to V are associated with different two-phonon processes, in which the emission occurs at the band edge.
- The horizontal black bands, crossing the map, denote hot luminescence processes associated with the different phonon branches.

In this study, photoluminescence measurements were carried out on different samples of DNA-wrapped single wall carbon nanotubes for 24 laser excitation energies in the near IR. A number of strong PL emission spots were identified with different channels of excitation and relaxation for a (6.5) nanotube, including one phonon, two phonon, hot luminescence processes, as well as radiative and non-radiative energy transferring processes between neighboring nanotubes, over a wide range of excitation and emission energies. A two dimensional (2D) excitation vs. emission spectral map obtained experimentally is shown on the left, whereas the schematics of the strongly emitting states are plotted on the right. I through V denote two-phonon processes associated with band edge emission, whereas VI denotes a first order, Raman-like process. The transitions going across the map horizontally denote hot luminescence processes and energy transfer between neighboring nanotubes associated with each of the phonon branches I through VI. The narrower transition (orange dotted line) going diagonally across the map denotes a resonance Raman scattering process associated with three different phonons. The study shows that the electronic relaxation processes observed in PL can be used to probe different physical interactions between photons, electrons, and phonons that are difficult to separately identify in most solid state systems.

The advance in this study is of interest both to researchers engaged in studies on carbon nanotubes and of optical processes in solids more generally.